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To: E. B. Sanders Date: October 30, 1981
From: R. A. Kornfeld
Subject: Plans and Objectives for the Chemical Research Instrumentation
Section for 1982.

This memo outlines the plans and objectives of the Chemical Research Instrumentation Section for 1982. The responsibilities of the section are to:

1. Provide an analytical resource for collaborative research and service requests in the areas of mass spectrometry, gas chromatography/mass spectrometry, pyrolysis, and laboratory data acquisition.
2. To ensure that future needs are met by improvements to currently available equipment and methodology as well as the purchase of new equipment.

In addition to handling the submission of samples on an as needed basis, several ongoing programs will be using the facilities:

1. Materials Evaluation (ongoing)

Materials that come in contact with cigarette components have been screened for the production of potentially undesirable compounds by using pyrolytic techniques. If initial screening methods are inconclusive, the sample is subjected to pyrolysis/GC/MS analysis. These analyses will continue in 1982.

2. Flavor and Flavor-Release Screening (ongoing)

As part of the screening protocol for flavor additives to tobacco, candidate compounds are subjected to pyrolysis/GC/MS analysis so that toxicity of any thermal decomposition products can be assessed. Volatile products will be identified using equipment in the section.

3. Aza-arenes from Nicotine Decomposition

The principal function for mass spectrometry in this project is the identification of selected aza-arenes in cigarette smoke. This endeavor will involve reproducing chromatographic patterns obtained by other investigators, obtaining GC/MS profiles, identifying candidate aza-arenes, and determining if other compounds are coeluting with these aza-arenes.

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Plans for instrument modification are as follows:

1. Uses for DuPont GC/MS System

Because of the limitations in its scan speed, the DuPont GC/MS system will be used only for requests involving packed column analysis. The major uses for this system are forecast to be:

- a. the identification and structure confirmation of synthesized compounds.
- b. the on-line analysis of pyrolytic products from routine requests when the DuPont has pyrolysis capability (1st Quarter).
- c. other analyses that can be satisfied using packed columns.

There will be a pilot program started in 1982 that will involve the use of the DuPont system by trained individuals other than section personnel. The training program will involve identifying individuals interested in using the DuPont GC/MS, training these scientists, monitoring their progress, and then allowing them to use the system. Of course, parts of the system that are easily susceptible to damage will be handled by section personnel. After the system is running well, the operator training program will begin (2nd Quarter).

2. Uses for the Finnigan GC/MS System

The principal functions for the Finnigan GC/MS systems are:

- a. to process requests requiring the use of capillary GC techniques.
- b. to participate in projects that require more complicated analysis than would be handled using the DuPont system.

Both of these responsibilities relate to the Finnigan system being used more in a research function. There are several modifications that will increase the capability of this instrument.

First change involves replacement of the data system to allow for both faster processing of spectra and greater capability

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for computerized file search of reference spectra. Additionally, the updated computer allows for simultaneous collection of data and processing of information from a separate data file. With the approval of the capital expenditure in 1981, this system will be functional by 2nd Quarter, 1982.

A second project is the installation of pyrolysis/capillary GC capability on the Finnigan system. The coupling of pyrolysis equipment with capillary columns will provide a powerful tool for studying the thermal decomposition of systems such as cooked flavors, Amadori compounds, aza-arene precursors, and flavored tobacco. This modification will be completed by the third quarter.

The other modification to be undertaken in 1982 is the insertion of a split between the GC and MS. The split will result in the ability to detect a minor component coeluting with a major one. Two specific detectors that could be attached to the split are a nitrogen selective detector or a radioactivity detector. The former detector would be useful for studies involving cooked flavors, nitrogen-containing flavors in smoke, and aza-arenes. The latter detector would serve to provide direct confirmation of the identity of radio-labelled material instead of relying on an unchanging chromatographic pattern from radio GC to GC/MS. This modification will be completed by the 3rd quarter.

Plans for laboratory data acquisition for the Chemical Research Division involve discussions about the type of data collection network, the specific needs of the various projects, and the type of system to purchase. These subjects will be discussed in conjunction with the search for a scientist to head the acquisition and installation of such a system.

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